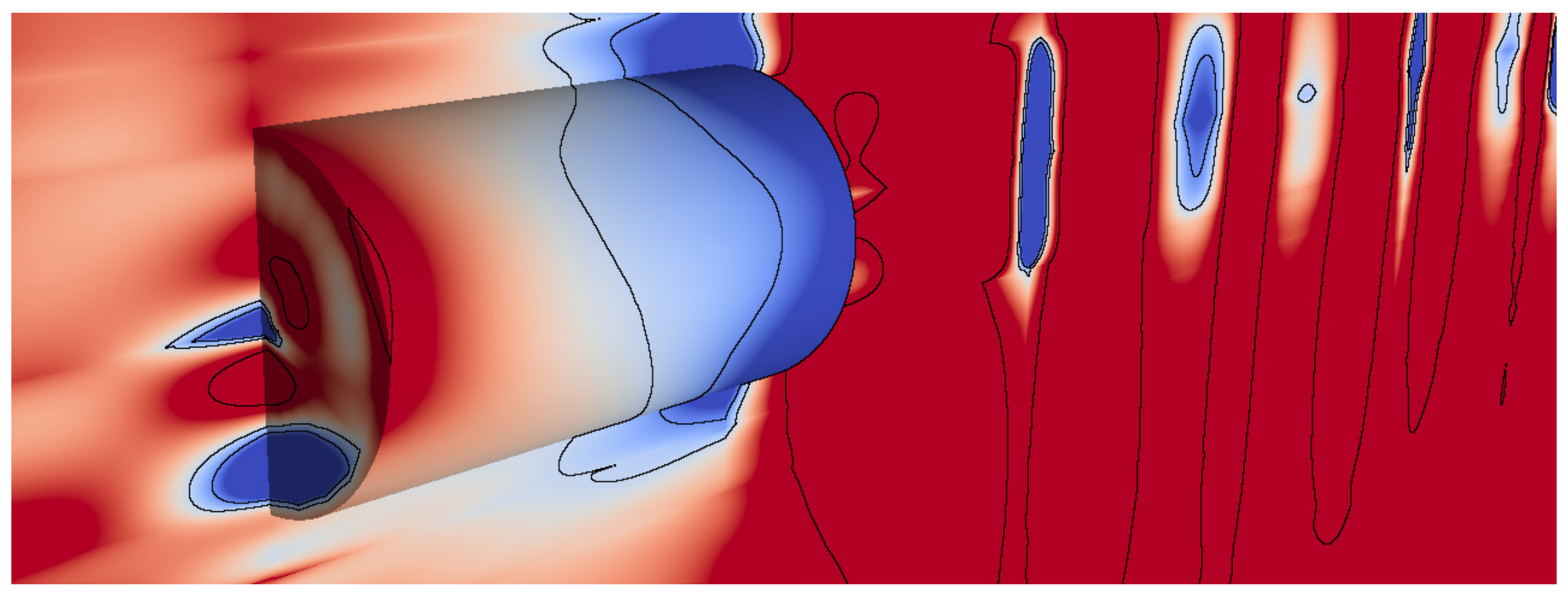
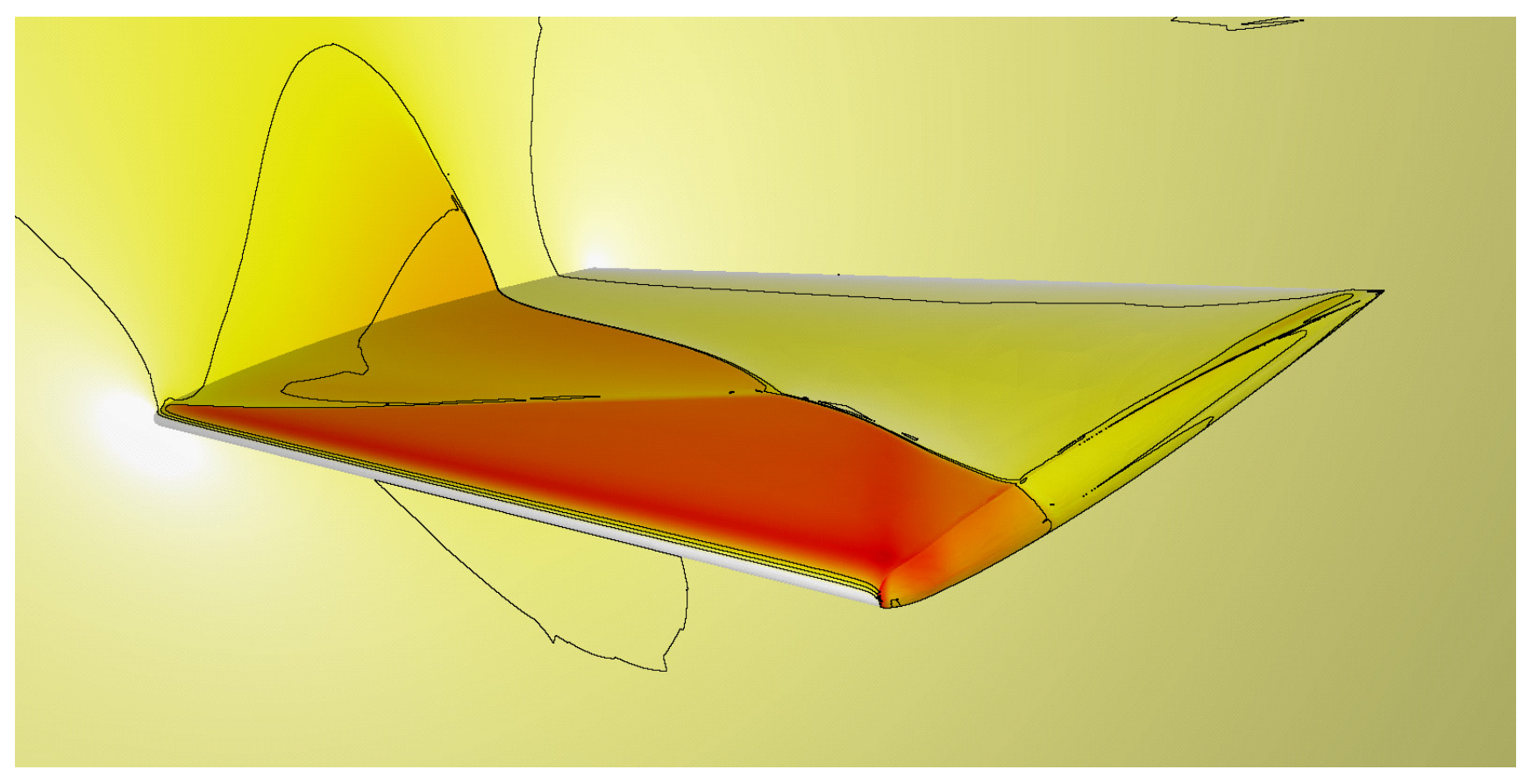
# Unconventional and Renewable Energy Research Utilizing Advanced Computer Simulations

## Science-based simulations on present GPUs and future extensions

We develop technologies for supporting finite element simulations on multicore streaming processors. The upward trends in graphics processor (GPU) performance are impressive, even relative to progressively more powerful, conventional CPUs. The SCI institute leverages its considerable track record and expertise in scientific computing on GPUs to pursue the development of new technologies and algorithms for finite element simulations on GPU clusters. Thus work takes place in the context of the NVIDIA Center of Excellence at the University of Utah and the SCI Institute.

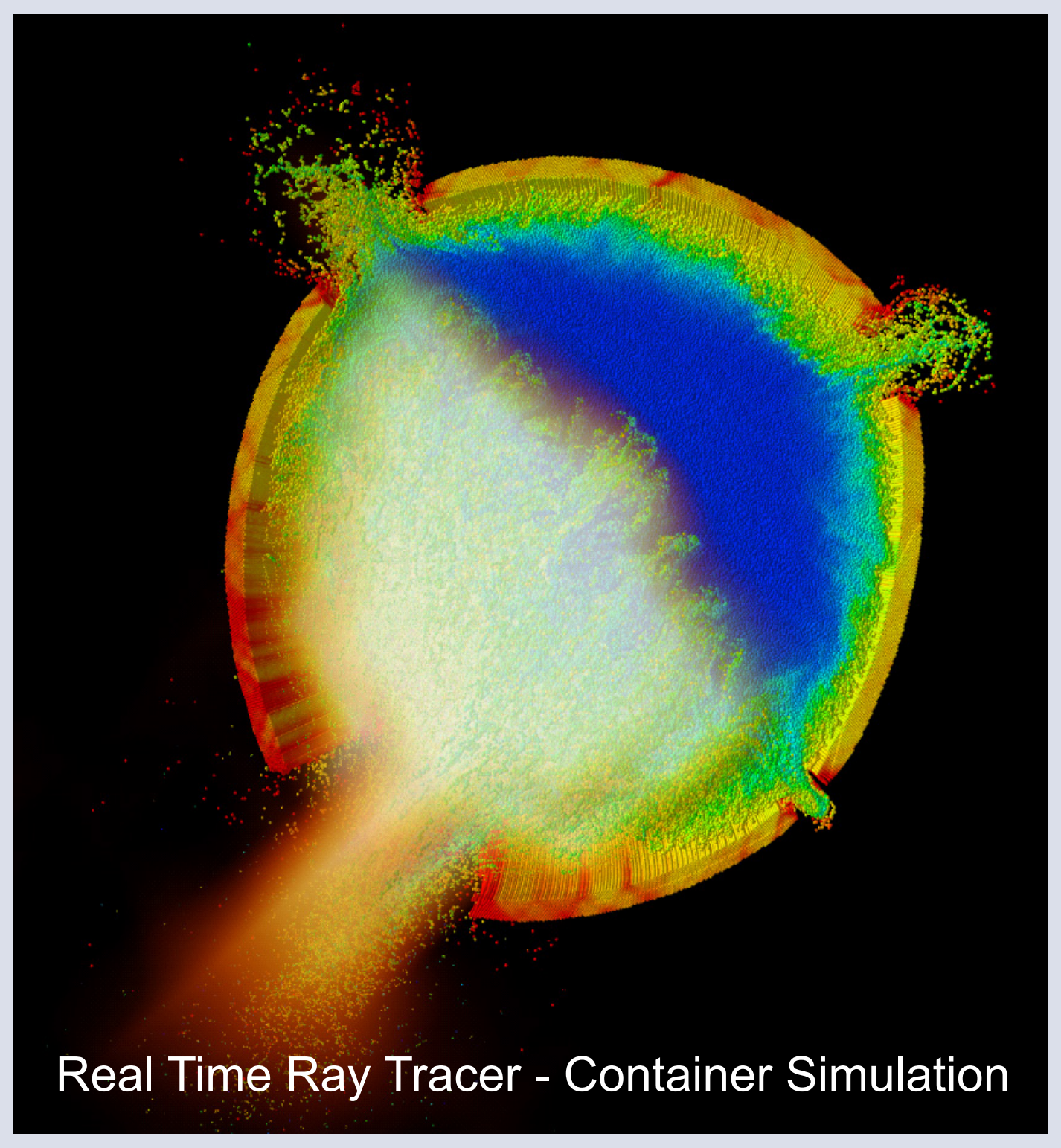


*View of the pressure field of a rotating canister moving through an incompressible fluid. A color map of the field, along with contours of constant pressure, have been applied to the cylinder and the cut-plane.*



*Mach number on the ONERA M6 Wing, rendered using ElVis (a system for the accurate and interactive visualization of high-order finite element solutions) and illustrating the application of color maps and contour lines on curved and planar surfaces.*

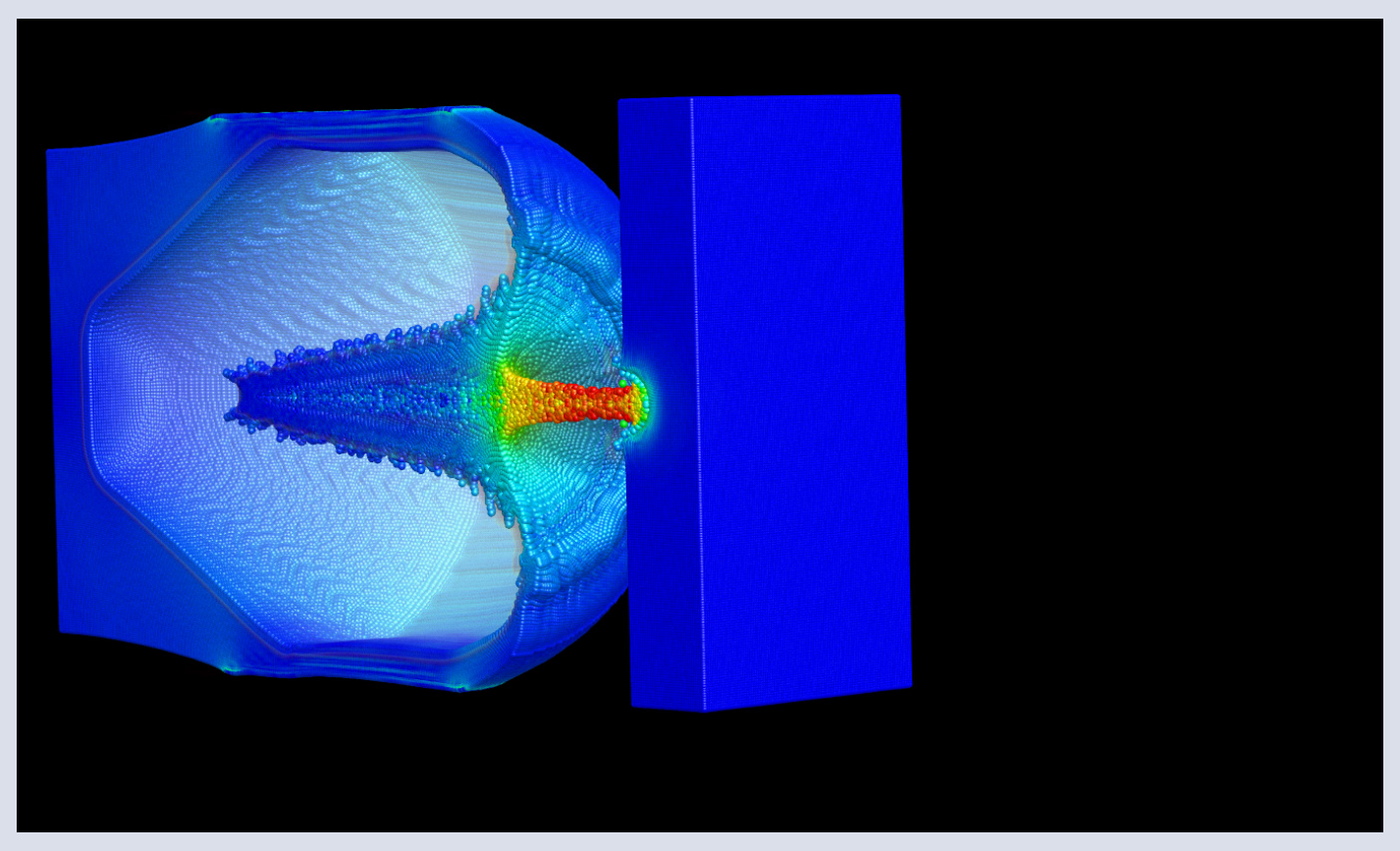
## Extending Uintah



Uintah is a parallel software environment for solving large-scale computational mechanics and fluid dynamics systems, and has particular strengths when dealing with systems that require large deformations, fire simulation, and fluid-structure interactions.

Uintah's general-purpose, fluid-structure interaction code has been used to characterize a wide array of physical systems and processes encompassing a wide range of time and length scales scientific problem-solving environment to simulate large multi-scale, multi-physics science-based energy systems.

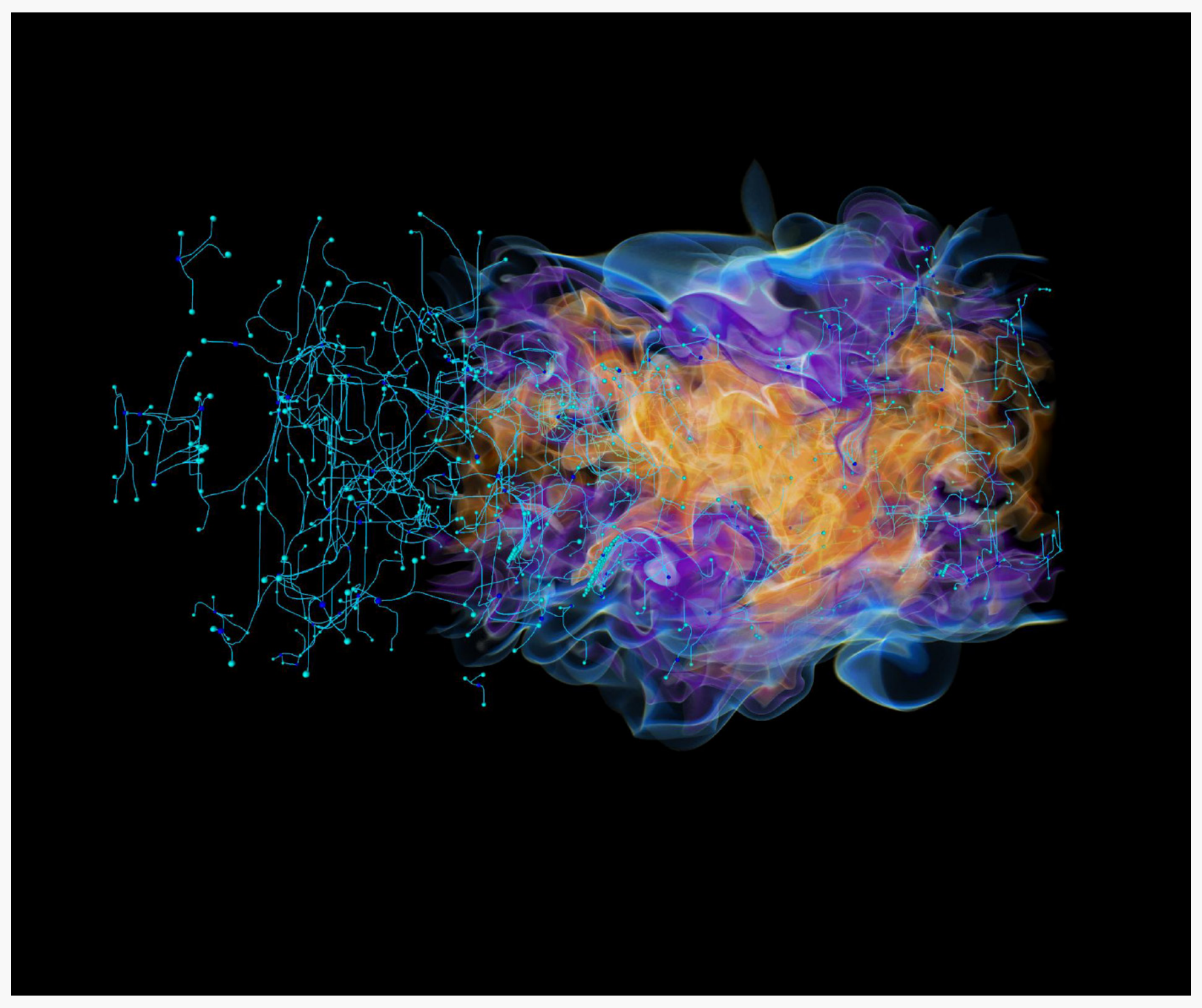
The broad applicability of Uintah makes it suitable for a range of energy problems such as flow through micro and nano-scale porous media as well as combustion examples related to flares, boilers and fires. The aim of the Uintah work is to show that Uintah may be used to solve challenging energy-related problems on large scale high-performance computers such as the Jaguar XT5 and the new Titan XK6 at Oak Ridge National Laboratory.



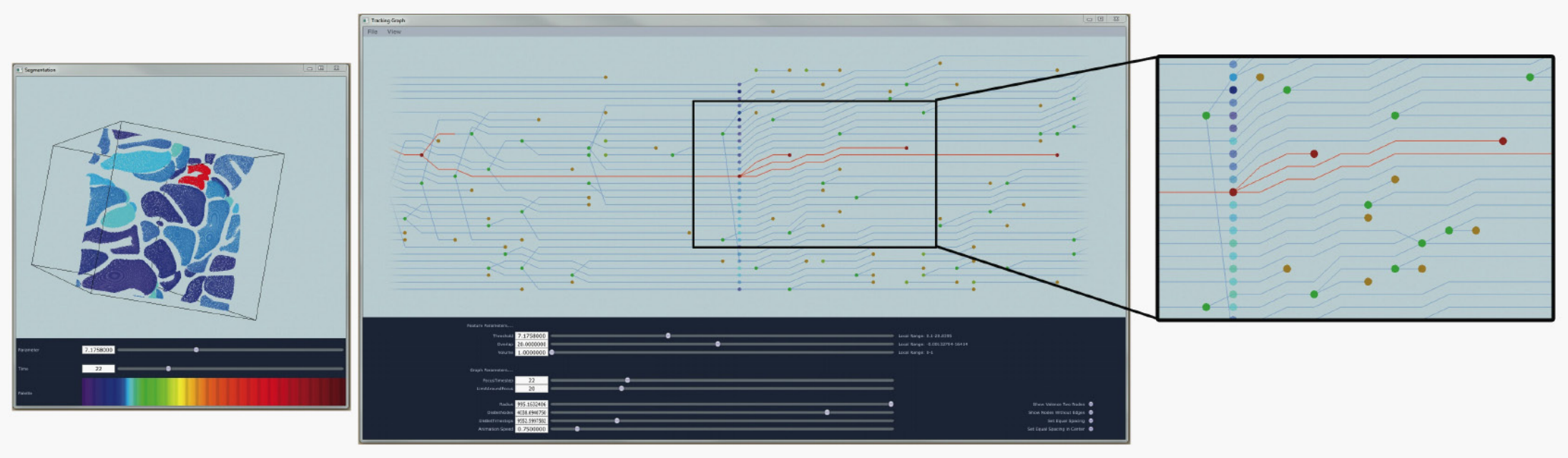
*Simulation of a shaped charge detonating, forming a jet which begins to penetrate a steel target. Particles are colored by velocity magnitude. The simulation was performed on the Ranger server using 1024 processors. Run time was approximately 2 days.*

## Large-scale visualization techniques for science-based energy system simulation applications

One of the greatest scientific and engineering challenges of the twenty-first century is to understand and make effective use of this growing body of information. Visual data analysis, facilitated by interactive interfaces, enables the detection and validation of expected results while enabling unexpected discoveries in science. The SCI Institute is an international leader in visualization, leveraging and expanding our expertise in large-scale visualization research and development toward the seamless integration of high-end visualization techniques with simulation results of energy systems.



*Left: Combustion accounts for the majority of the world's energy needs, and scientists are developing increasingly large and complex simulations to gain a better insight into clean and efficient fuels and burning devices. Visualization and analysis algorithms are integral to answering science questions about combustion; however, these algorithms must be executed concurrently with the simulations without negatively impacting their performance. Recent results show how in-situ and in-transit paradigms are used to achieve efficient topological analysis and high resolution visualizations that are well coupled with combustion simulation via high-throughput data movements that minimize any performance overhead.*

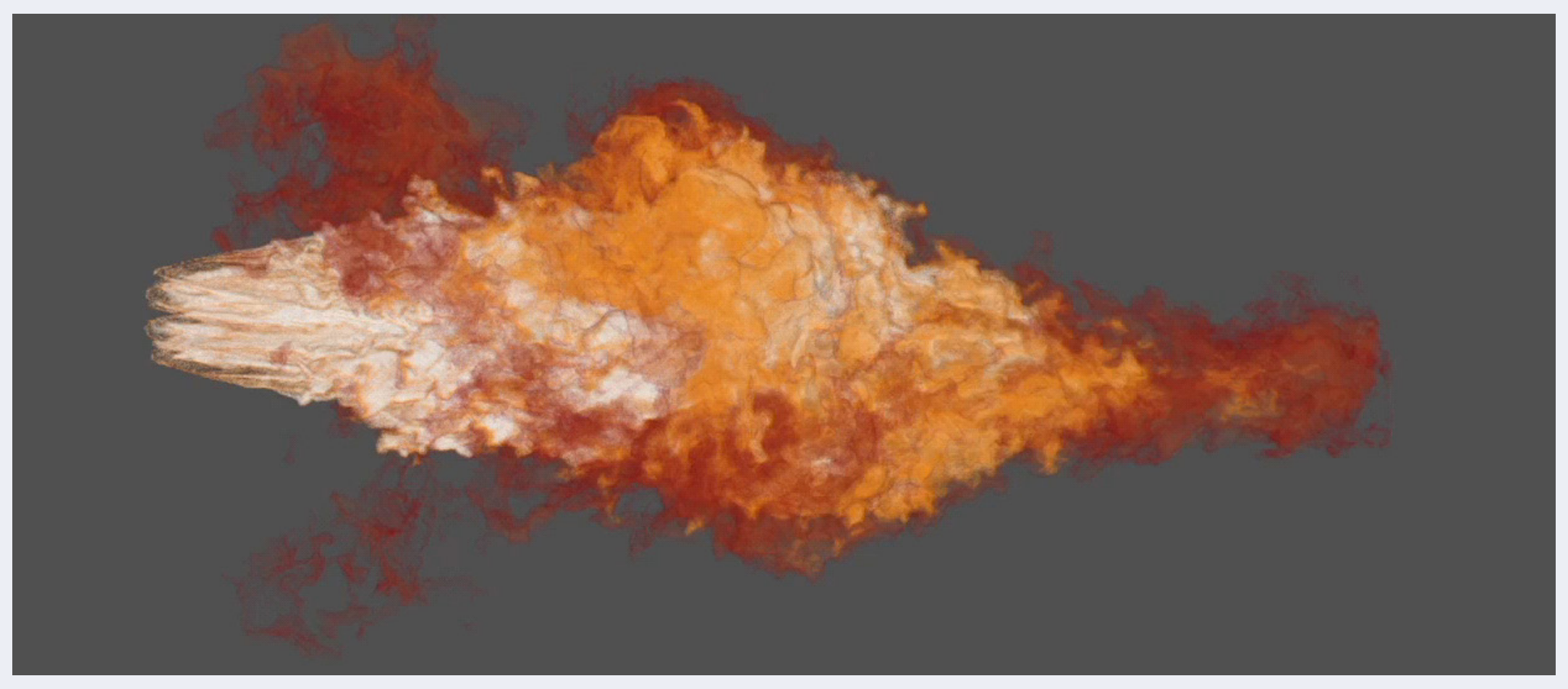


Above: Tracking graphs track the evolution (creation, merging, splitting, death) of pre-computed feature hierarchies, selects features interactively. They are linked with segmentation viewer and modify interactively feature definition parameters.

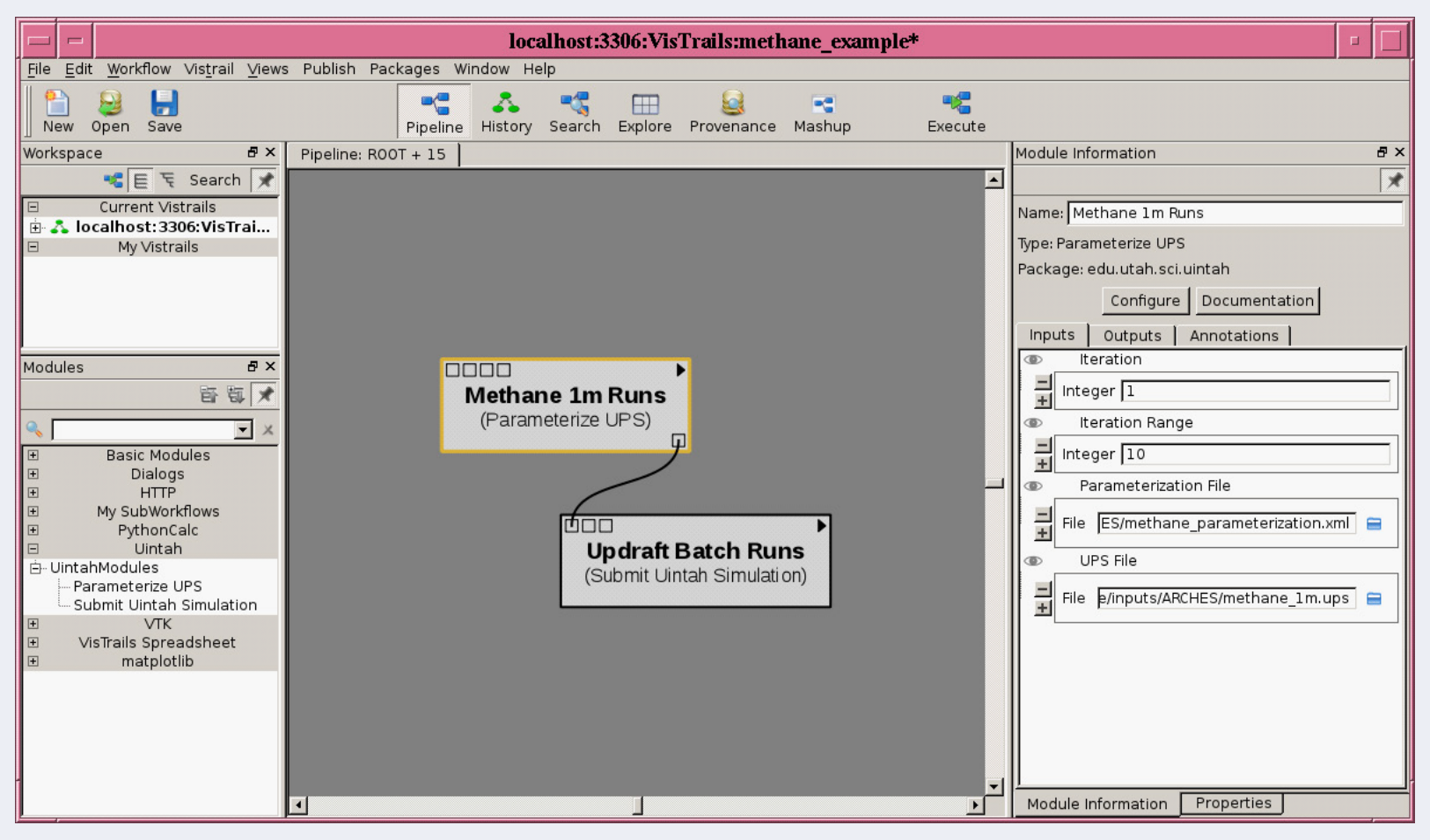
## Provenance enabling Uintah:

Exploration of large-scale scientific systems using computational simulations produces massive amounts of data that must be managed and analyzed. Because of the volume of data manipulated, and the complexity of the simulations and analysis workflows it is crucial to maintain detailed provenance (i.e., an audit trail) of the derived results. Provenance is necessary to ensure reproducibility as well as enable verification and validation of the simulation codes and results.

In order to manage large-scale simulations and the analysis of their results, we build upon and substantially extend VisTrails, an open-source provenance management and scientific workflow system. A distinguishing feature of the VisTrails system is a comprehensive provenance infrastructure that maintains detailed information about the steps followed and data derived in the course of an exploratory task.



*Volume rendering of temperature for the IFRF FOSPER furnace firing natural gas with a CO2/O2 mixture. This is an example of the type of simulation that lends itself to a parameter study for validation purposes.*

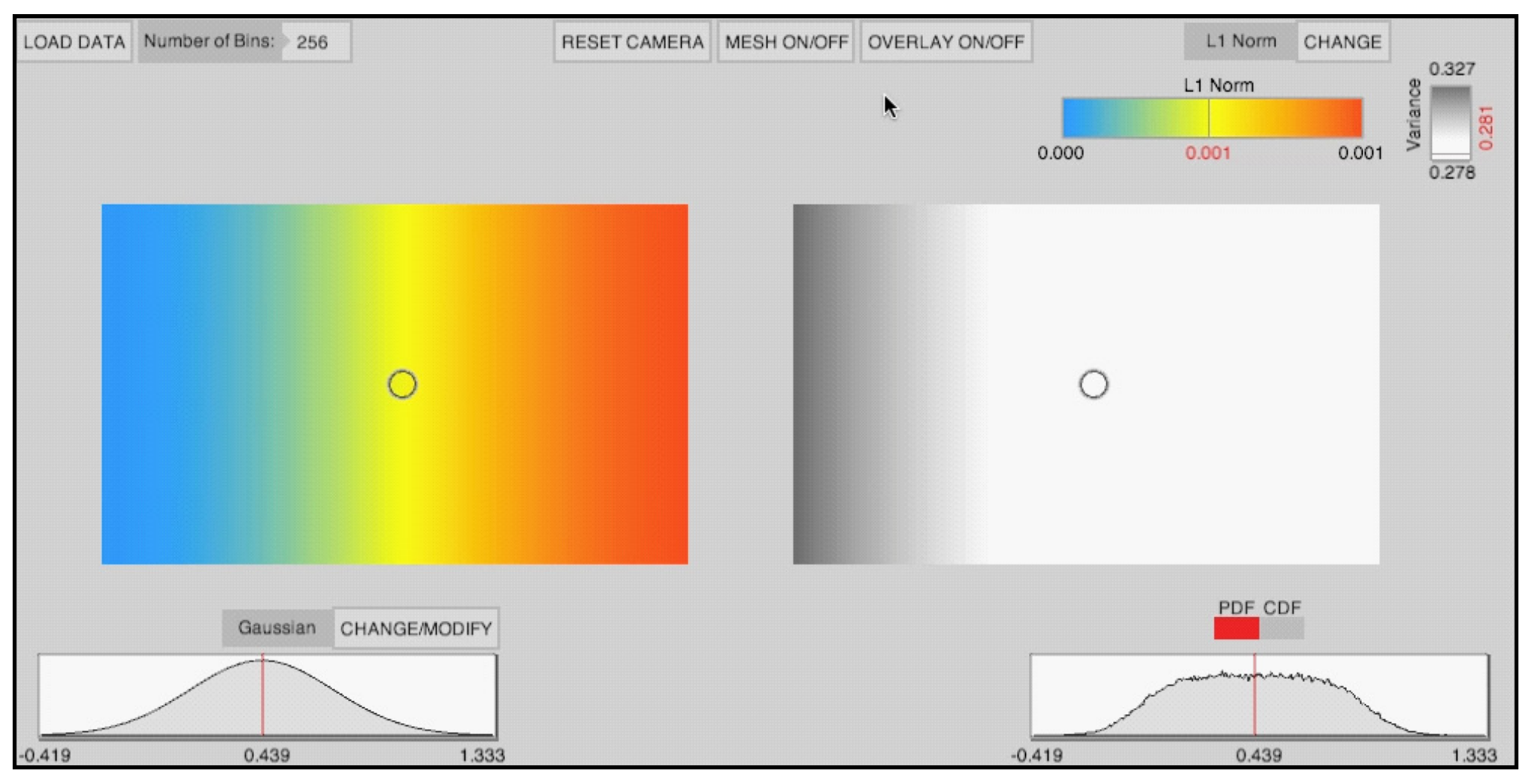


*Uintah parameterization batch execution prototype In VisTrails.*

## Uncertainty estimation and visualization

With large computational simulations there is substantial uncertainty inherent in any prediction of science-based systems. A number of factors contribute to uncertainty, including experimental measurements, mathematical formulation, and the way different processes are coupled together in the numerical approach for simulation. Tracking of and analysis of this uncertainly is critical to any work that will truly impact the creation of future energy systems.

ProbVis, a visualization and exploration tool for probability distribution functions developed at the SCI Institute, allows for the interactive display and exploration of a spatial collection of data distributions.



Exploration tool for exploring probability distribution functions across the spatial domain. Uncertainty is encoded as a PDF at each grid point. The tool uses a distance metric to compare each PDF to a user-specified canonical PDF and this metric is visually encoded using a colormap. The tool allows a user to immediately compare the shape of all PDFs in the dataset, a task which previously required users to individually explore each location, or summarize the data with statistics that assumed Gaussian distributions.

## Future Directions:

Visualization of Geologic Materials - Volume rendering of CT X-Ray of a large rock sample, complex fracturing test conducted by TerraTek, under deep earth stress conditions. The created fracture (visualized in red) interacts with a large Calcite mineral inclusion (show in gold). This image allows visualization of the fracture resistance provided by the Calcite inclusion. The fracture width is about 1 mm and the inclusion is 30-50 mm in dimension. (The X-Ray voxel size is 1.00 mm by 0.17 mm by 0.17 mm.)